Electronic Supplementary Information

Table S1. Calculated J values, considering a model with twenty-one J values, for one of the two molecules (a' and a'', see Fig. 2) of the Fe_9 dimer using numerical calculations (double-ζ basis set only triple-ζ for iron atoms) with Siesta code[6] and PBE functional[7] and with NWChem code[8] using an all electron triple-ζ basis set[9] and the B3LYP functional.[10] The label of the J value indicates the two interacting metal centers (see Fig. 1).

J (cm^{-1})	bridging ligand	a' Siesta	a'' Siesta	a'' NWChem
J_{23}	2 μ_3-OH, μ_2-O_2CPh	-1.3	-1.3	-1.4
J_{12}	μ_3-O, μ_3-OH, μ_2-O_2CPh	-15.2	-15.3	-13.3
J_{34}	μ_3-O, μ_3-OH, μ_2-O_2CPh	-16.5	-16.5	-14.8
J_{13}	μ_3-OH	-21.0	-21.0	-24.5
J_{24}	μ_3-OH	-20.0	-20.0	-22.4
J_{28}	μ_3-O, μ_2-O_2CPh	-50.1	-50.0	-67.4
J_{36}	μ_3-O, μ_2-O_2CPh	-58.8	-59.5	-77.3
J_{18}	μ_3-O	-42.7	-42.7	-63.5
J_{46}	μ_3-O	-40.2	-40.4	-57.4
J_{16}	μ_3-OH	-18.2	-18.1	-22.8
J_{48}	μ_3-OH	-14.2	-14.1	-17.7
J_{67}	μ_3-O, μ_3-OH	-4.7	-4.7	-4.3
J_{78}	μ_3-O, μ_3-OH	-10.1	-10.1	-9.6
J_{56}	μ_3-O, μ_2-O_2CPh	-49.5	-49.3	-67.2
J_{89}	μ_3-O, μ_2-O_2CPh	-48.3	-48.1	-63.0
J_{17}	μ_3-OH	-13.3	-13.2	-17.4
J_{47}	μ_3-OH	-10.7	-10.7	-12.8
J_{45}	μ_3-O	-29.4	-28.7	-34.7
J_{19}	μ_3-O	-27.0	-27.0	-31.7
J_{57}	μ_3-O, μ_2-O_2CPh	-47.7	-47.7	-64.6
J_{79}	μ_3-O, μ_2-O_2CPh	-49.8	-49.9	-67.2